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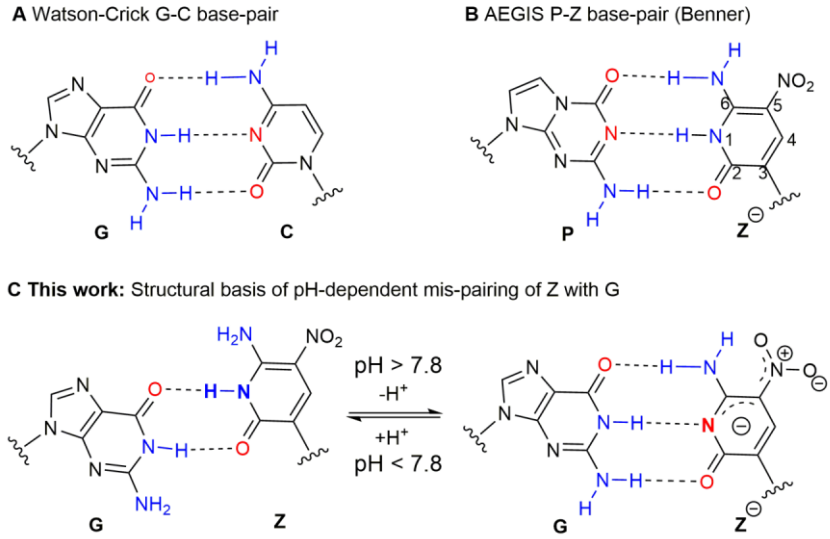


Figure 1. Base-pairs of (A) naturally-occurring G-C, (B) P-Z and (C) the pH-dependent G-Z mispair.

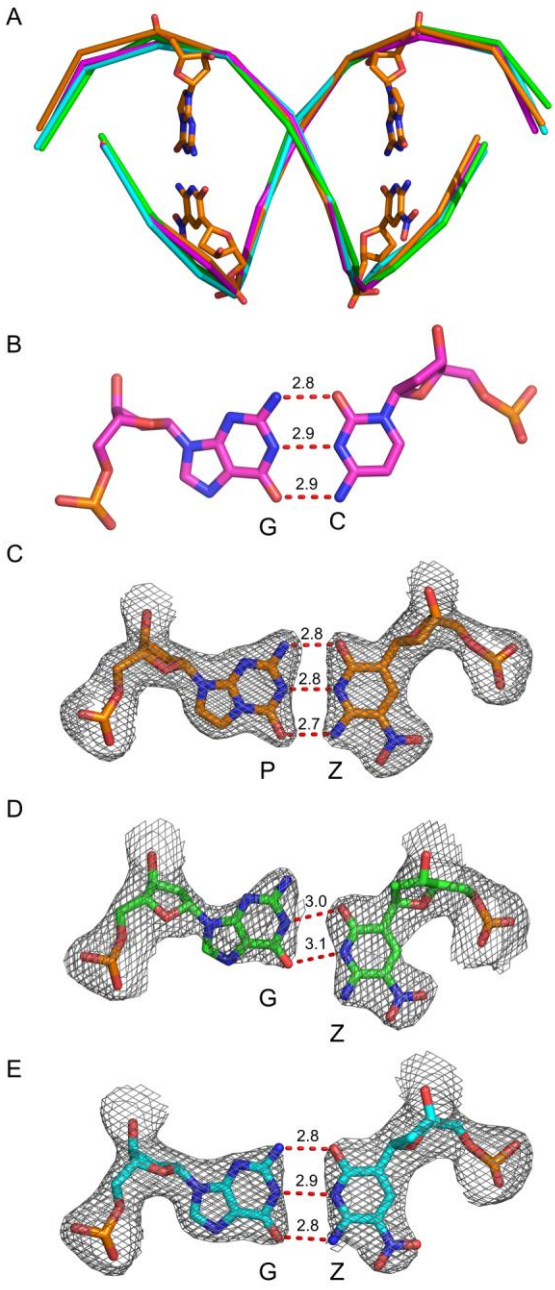


Figure 2. (A) Overlay of ODN1 (magenta), ODN2 (orange), ODN3a (green) and ODN3b (cyan) crystal structures. Base-pairs for the 4-position (B) G-C (ODN1), (C) P-Z (ODN2 at pH 7.0), (D) G-Z (ODN3a at pH 7.8), and (E) G-Z (ODN3b at pH 8.5). Hydrogen-bond distances shown in Ångstroms. The $2F_o$-F_c electron density is contoured at 1.0σ.

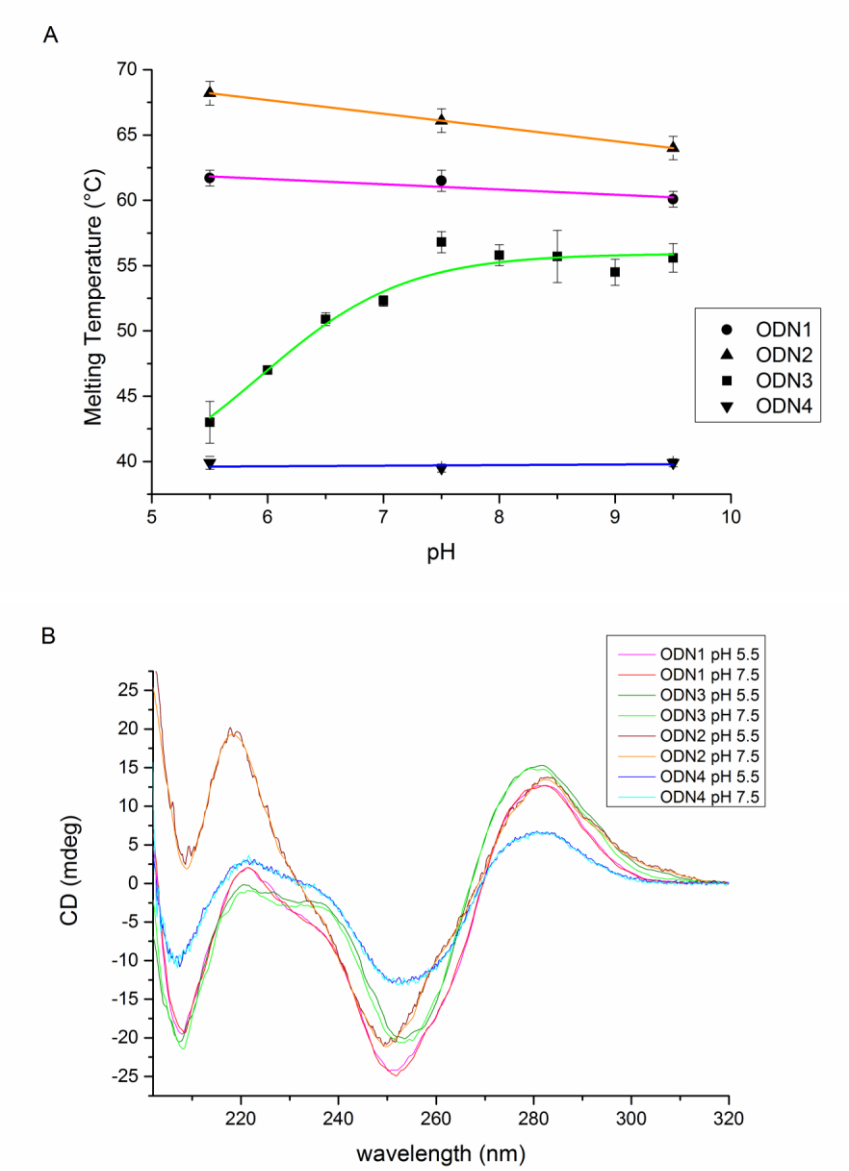


Figure 3. Comparative analysis of duplex stability and conformation of ODN1-4. (a) UV-vis melting temperatures of ODN1-3 duplexes between pH 5.5 and 9.5 measured at 260 nm. (See also Fig. S9-28, Table S2-3) (b) CD spectra of ODN1-3 at pH 7.5 exhibit characteristic right-handed B-type DNA spectra. (See also Fig. S29-34)

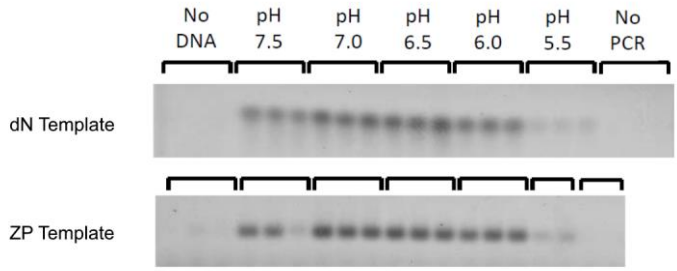


Figure 4. The effect of pH on PCR amplification of a DNA template containing a single P-Z base pair compared to a DNA template containing no P and Z nucleotides. Each PCR was conducted in cacodylate buffer. (See also Fig. 35-37)

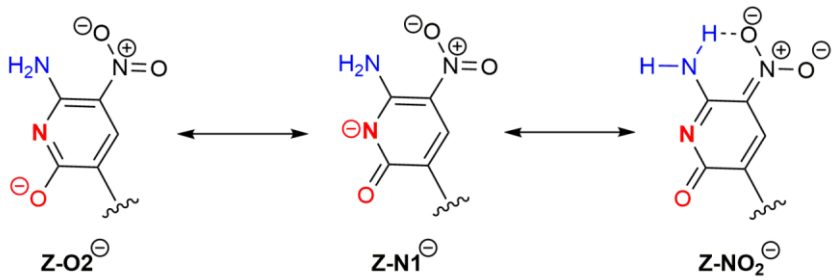
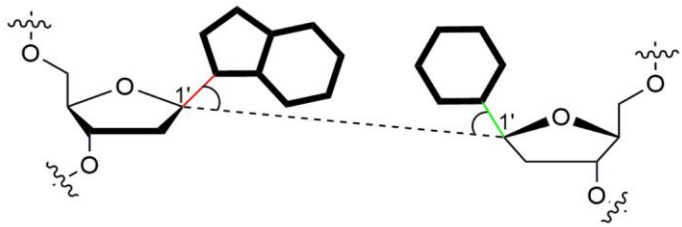


Figure 5. Putative resonance structures of the Z anion.

Table 1. Schematic representation of a purine-pyrimidine base-pair in position 4.



	C-1′-C-1′ Distance (Å)	N-9-C-1′-C-1′ Angle (°)	N-1(C-1)-C-1′-C-1′ Angle (°)	Angle of C-1′-C-1′ vector (relative to ODN1) (°)
ODN1[a]	10.4	56.5	55.9	0
ODN2	10.8	55.5	52.3	2.3
ODN3a	10.7	44.5	63.0	9.6
ODN3b	10.8	57.5	54.7	1.0
ODN4[b]	10.4	42.5	69.9	14.0

Table legend.
[a]PDB ID 463D
[b]PDB ID 113D